PROPOSAL

Syllabus

1) Prof. Federico Totti & Dr. Matteo Briganti

University of Florence, federico.totti@unifi.it & matteo.briganti@unifi.it

-CV (1-2 pag) + picture

-Bibliometric data: h-index 30 (Scopus), 30 (WoS). Citations: 3477 (Scopus), 3403 (Wos)

h-index 12 (Scopus), 11 (WoS). Citations: 337 (Scopus), 331 (Wos)

-Selection of the 10 most relevant publications and/or patents

1) A. Patrascu, S. Calancea, M. Briganti, S. Soriano, A. M. Madalan, R. A. Allão Cassaro, A. Caneschi, F. Totti, Maria G. F. Vaz, M. Andruh **Chemical Communications**, **2017**, 53, 6504-6507.

2) Malavolti, M. Briganti, M. Hänze, G. Serrano, I. Cimatti, G. McMurtrie, E. Otero, P. Ohresser, F. Totti, M. Mannini, R. Sessoli, and S. Loth **NanoLetters**, **2018,** 18, 7955–7961.

3) M. Briganti, G. Fernandez Garcia, J. Jung, R. Sessoli, B. Le Guennic, and F. Totti **Chemical Science**, **2019**, 10, 7233-7245.

4) A. Patrascu, M. Briganti, S. Soriano, S. Calancea, R. A. Allão Cassaro, F. Totti, M. G. F. Vaz, , M. Andruh **Inorganic Chemistry, 2019**, 58, 13090-13101.

5) Serrano, L. Poggini, M. Briganti, A. L. Sorrentino, G. Cucinotta, L. Malavolti, B. Cortigiani, E. Otero, P. Sainctavit, S. Loth, F. Parenti, A.-L. Barra, A. Vindigni, A. Cornia, F. Totti, M. Mannini and R. Sessoli **Nature Materials, 2020**, 19, 546–551.

6) L. C. de Camargo, M. Briganti, F. S. Santana, D. Stinghen, R. R. Ribeiro, G. G. Nunes, J. F. Soares, E. Salvadori, M. Chiesa, S. Benci, R. Torre, L. Sorace, F. Totti, and R. Sessoli **Angewandte Chemie Int. Ed., 2021**, 60, 2588–2593.

7) M. Briganti, E. Lucaccini, L. Chelazzi, S. Ciattini, L. Sorace, R. Sessoli, F. Totti, and M. Perfetti **Journal of the American Chemical Society, 2021**, 143, 8108–8115.

8) Matteo Briganti and Federico Totti. **Dalton Transactions, 2021**, 50, 10621-10628. (invited)

9) M. Briganti, F. Santanni, L. Tesi, F. Totti, R. Sessoli, A. Lunghi **Journal of the American Chemical Society, 2021,** 143, 13633–13645.

10) Matteo Briganti, Federico Totti, Marius Andruh. **Dalton Transactions, 2021**, 50, 15961-15972. (invited)

2) Title of the course

ORBITAL INTERACTIONS IN CHEMISTRY: FROM THEORY TO SIMPLE SYSTEMS.

3) Course content detailed per lesson of 2 h (possibly with dates and room real and virtual)

First lesson. Atomic orbitals. Variational Theorem. Overlap integrals. Secular equations and determinants. Two orbital problem (degenerate and non-degenerate case).

Perturbational atomic orbitals theory. Orbital Interaction diagrams. Three orbital problem, degenerate and non degenerate case. Hybridization.

Second lesson. Group theory. Point groups. Character tables and irreducible representations. Projection operators. Symmetry adapted Linear Combination of Atomic Orbitals. Symmetry properties of integrals.

Third lesson. How to build molecular orbitals for AH_2 systems: $D_{\infty h}$ and C_{2v}; Orbital correlations; Electronegativity considerations; Walsh diagrams; Jahn-Teller distortions.

Forth lesson: H_3 system: $D_{\infty h}$ and $D_{3h:}$ H_4 system: D_{2h}, D_{4h}, and T_d; H_6 and AH_6 system: D_{6h} and D_{3h}.

4) Course program (150-200 words)

The course will cover the construction of molecular orbital interactions through a perturbative theoretical approach. In this framework, the operative applications will cover both organic and inorganic species. The aim of the course is to make the student able to sketch the electronic structure of the species under study in order to understand and predict their electronic properties and reactivity.

5) Suggested reading

ALBRIGHT T.A.; BURDETT J.K.; WHANGBO M.-H. Orbital Interactions in Chemistry, 2nd edition, John Wiley & Sons, Inc., 2013.

BERSUKER I.B., Electronic Structure and Properties of Transition Metal Compounds, 2nd edition, John Wiley & Sons, Inc., 2010.

6) Learning Objectives

Construction of molecular orbital interactions through a perturbative theoretical approach in order to make the student able to sketch the electronic structure of the species under study, understand and predict their reactivity and electronic properties. Introduction of different theoretical methods to compute electronic, spectroscopic and magnetic properties of molecule-based materials.

7) Knowledge and skills to be acquired

Perturative MO approach; Orbital interaction diagrams; Rationalization of physico-chemical properties in terms of electronic structure

8) Prerequisites

Basic knowledge of the most common quantum chemical methods to simulate the electronic structure of molecules: Hartree-Fock, Density Functional Theory.

9) Teaching Methods

Frontal lessons and practical exercises. Each student should use its own computer.

10) Further information

11) Type of Assessment: oral test (Discussion about the building of orbital interaction diagram of simple chemical systems). The final evaluations will have to be validated maximum 1 month after the end of the course

Total hours must be: 8 h frontal lessons (3 ECTS)

Period:

Indicatively on May-June